

1,2-Naphthalenedione, 3,8-dimethyl-5-(1-methylethyl)-
5574-34-5 | DTXSID80204286

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 2200 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.12e-01

Confidence level: 6.70e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Acetylaminofluorene</div> <div>Measured: 1380</div> <div>Predicted: 1860</div>	<div>Image not found</div> <div>9-Anthracenecarboxylic acid</div> <div>Measured: 550</div> <div>Predicted: 1400</div>	<div>Image not found</div> <div>9-Anthracenemethanol</div> <div>Measured: 4070</div> <div>Predicted: 5400</div>
<div>Image not found</div> <div>Anthraquinone</div> <div>Measured: 3720</div> <div>Predicted: 2300</div>	<div>Image not found</div> <div>Pendimethalin</div> <div>Measured: 5010</div> <div>Predicted: 4980</div>	